Scaling of Self-Avoiding Walks in High Dimensions

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Abstract

We examine self-avoiding walks in dimensions 4 to 8 using high-precision Monte-Carlo simulations up to length $N = 16384$, providing the first such results in dimensions $d > 4$ on which we concentrate our analysis. We analyse the scaling behaviour of the partition function and the statistics of nearest-neighbour contacts, as well as the average geometric size of the walks, and compare our results to $1/d$-expansions and to excellent rigorous bounds that exist. In particular, we obtain precise values for the connective constants, $\mu_5 = 8.838544(3)$, $\mu_6 = 10.878094(4)$, $\mu_7 = 12.902817(3)$, $\mu_8 = 14.919257(2)$ and give a revised estimate of $\mu_4 = 6.774043(5)$. All of these are by at least one order of magnitude more accurate than those previously given (from other approaches in $d > 4$ and all approaches in $d = 4$). Our results are consistent with most theoretical predictions, though in $d = 5$ we find clear evidence of anomalous $N^{-1/2}$-corrections for the scaling of the geometric size of the walks, which we understand as a non-analytic correction to scaling of the general form $N^{(4-d)/2}$ (not present in pure Gaussian random walks).

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1 Introduction

The universal properties of linear flexible polymers in a dilute solution can be modelled by the lattice model of self-avoiding walks (SAW), and have been studied for this purpose [1] for over 50 years [2]. Being described by the limit $n \to 0$ of the O(n) ϕ^4 field theory [3, 4] places SAW amongst the most fundamental models in statistical physics along with the Ising ($n = 1$) and Heisenberg ($n = 3$) models, while its description as a non-Markovian random walk makes it of intense interest to mathematicians [5]. SAW are also of interest to the combinatorial mathematician as a fundamental combinatorial problem. As a critical phenomenon, in the context of theoretical physics, the limit of the length of the walk going to ∞ can be thought of as equivalent to approaching a critical temperature (in a generating function approach the generating variable acts as the Boltzmann weight in an O(n) model). Results from the associated field theory [3, 4] and subsequent confirmation by numerical methods, including careful series analysis of exact enumerations [6, 7] and statistical analysis of high precision Monte Carlo simulations [8], indicate that the upper critical dimension for SAW is $d_u = 4$. Above this dimension it is expected that SAW behaviour is dominated by the same behaviour as occurs in Markovian random walks (in a renormalisation group analysis of the O(0) ϕ^4 field theory both models are controlled by the so-called Gaussian fixed point). We expect that while dominant exponents and ratios of scaling amplitudes are the same as for RW the self-avoidance constraint will affect scaling amplitudes and corrections to scaling. In addition, apparently asymptotic $1/d$-expansions give reasonable estimates of the connective constants. On the other hand, much is known on a mathematically rigorous level [9, 10, 11, 5], thanks to the ingenuity of the lace expansion, and so the similarity of pure random walk (RW) and SAW behaviour can be quantified precisely to some extent. Despite all this non-rigorous and rigorous information several aspects of SAW in high dimensions require numerical investigation. First, the connective (or growth) constants, while bounded by rigorous arguments and estimated by $1/d$-expansion values (and series analysis of fairly short exact enumerations), are not known precisely from Monte Carlo simulations, and so the relative value of different bounds is not well understood. Second, the corrections to scaling in high dimensions have not been investigated, and since controversies and intriguing findings occur [12] in low dimensions for the SAW and related models, it is of interest to clarify these in high dimensions. In any case, due to SAW being such a fundamental model it clearly is of interest for us to establish as complete a description of the behaviour of SAW as possible.

We have simulated self-avoiding walks on the d-dimensional hypercubic lattice in dimensions $d = 4$ to $d = 8$ using the Pruned-Enriched Rosenbluth Method (PERM), a clever generalisation of a simple kinetic growth algorithm [13, 14] using a combination of enrichment and pruning strategies to generate walks whose weights are largely distributed around the expected peak of the distribution. We have utilised an implementation similar to that described in [15], where the enrichment and pruning thresholds are dynamically changed in response to the output of the algorithm while maintaining a constant ratio between these thresholds. For each dimension

$d = 4, \ldots, 8$, we have generated 10^8 samples of length $N = 4096$ and 10^7 samples of length $N = 16384$. While not having completely independent samples we have crudely estimated the effect of the dependence and so are able to give error estimates for our values. The PERM algorithm is particularly appropriate for high-dimensional simulations where SAW are close to RW, which are simply generated by a Rosenbluth-Rosenbluth approach [16]. While our four-dimensional simulations build on the careful previous work of Grassberger *et al.* [8], who simulated SAW up to length 4000 on the four-dimensional hypercubic lattice, our higher dimensional simulations are without parallel. In $d = 4$, our simulations do not provide any further insight [8, 15] into the subtle logarithmic corrections predicted in four dimensions, but simply allow us to update the connective and other constants in that dimension with estimates that are an order of magnitude better than previously obtained. In dimensions $d > 4$, we compare our results to the bounds of the lace expansion and other approaches, to the $1/d$-expansion, and to series analysis of exact enumeration data. Our main results are contained in Tables 1, 2 and 3. Apart from the precision of our estimates, our other contribution is to point out evidence for anomalous sub-dominant corrections to scaling in five dimensions (which presumably occur in higher dimensions though so weakly as to be not practically measurably).

Let the number of self-avoiding walks on the lattice of interest be c_N, that is $c_N \equiv |\Omega_N|$ where Ω_N is the set of all self-avoiding walks φ of length N steps ($N+1$ sites) with one end at some fixed origin. Let p_N be the number of self-avoiding polygons (closed walks) of length N. In this paper we consider the d-dimensional hypercubic lattice for $d = 4$, 5, 6, 7 and 8. We define a reduced free energy or rather entropy per step κ_N as

$$\kappa_N = \frac{1}{N} \log c_N. \tag{1.1}$$

Let $\langle Q \rangle_N$ denote the simple average of any quantity Q over the ensemble set of allowed paths Ω_N of length N. Let $M(\varphi)$ be the number of non-consecutive nearest-neighbour contacts (pairs of lattice sites occupied by the walk) for a given walk φ. We define a normalised mean number of contacts m_N per step by

$$m_N = \frac{\langle M \rangle}{N}\,, \tag{1.2}$$

and a normalised fluctuation in the number of contacts per step by

$$f_N = \frac{\langle M^2 \rangle - \langle M \rangle^2}{N}\,. \tag{1.3}$$

For a SAW model where each configuration is weighted by a Boltzmann weight (say, $\omega^{M(\varphi)}$) to the number of nearest-neighbour contacts (this model is known as interacting SAW or ISAW) the quantities m_N and f_N are proportional to the internal energy and specific heat in the limit $\omega \to 1$. The thermodynamic limit for SAW is given by the limit $N \to \infty$ so that the thermodynamic limit entropy per step is given by

$$\kappa_\infty = \lim_{N \to \infty} \kappa_N\,. \tag{1.4}$$

Given the thermodynamic limit exists this quantity determines the partition function asymptotics, i.e. c_N grows to leading order exponentially as μ^N with the connective constant $\mu = e^{\kappa_\infty}$.

In our simulations we also calculated two measures of the walk's average size. Firstly, specifying a walk by the sequence of position vectors $\mathbf{r}_0, \mathbf{r}_1, ..., \mathbf{r}_N$ the average mean-square end-to-end distance is

$$\langle R_e^2 \rangle_N = \langle (\mathbf{r}_N - \mathbf{r}_0) \cdot (\mathbf{r}_N - \mathbf{r}_0) \rangle \ . \tag{1.5}$$

We shall use the symbol $R_{e,N}^2$ to be equivalent to

$$R_{e,N}^2 \equiv \langle R_e^2 \rangle_N . \tag{1.6}$$

The mean-square distance of the sites occupied by the walk from the endpoint $\mathbf{r}_0$ of the walk is given by

$$\langle R_m^2 \rangle_N = \frac{1}{N+1} \sum_{i=0}^{N} \langle (\mathbf{r}_i - \mathbf{r}_0) \cdot (\mathbf{r}_i - \mathbf{r}_0) \rangle \ . \tag{1.7}$$

Again we define

$$R_{m,N}^2 \equiv \langle R_m^2 \rangle_N . \tag{1.8}$$

Our main new results concern $d > 4$, so we shall now discuss the theoretical predictions for those dimensions. It has been proved [17] that the thermodynamic limit exists, ie. μ exists. Furthermore it has been proved in sufficiently high dimensions [9, 10] that

$$c_N = A \mu^N \left(1 + O(n^{-\epsilon})\right) \tag{1.9}$$

for any $\epsilon < \min\left((d-4)/2, 1\right)$ and

$$R_{e,N}^2 = d_e \, N \, \left(1 + O(n^{-\epsilon})\right) \tag{1.10}$$

for any $\epsilon < \min\left((d-4)/4, 1\right)$.

On the other hand on a non-rigorous level from the general theory of critical phenomena [18] we further expect that the numbers of walks and polygons have both analytic and non-analytic corrections to scaling:

$$c_N \sim A \mu^N N^{\gamma-1} \left(1 + \frac{w_a}{N} + \frac{w_e}{N^{\Delta_e}}\right) \tag{1.11}$$

and

$$p_N \sim A \mu^N N^{\alpha-2} \left(1 + \frac{p_a}{N} + \frac{p_e}{N^{\Delta_e}}\right) \tag{1.12}$$

with $\gamma - 1 = 0$ and $\alpha - 2 = -d/2$ for $d \geq 5$. From this we deduce that the entropy, mean number of contacts and their fluctuations scale as

$$\kappa_N \sim \kappa_\infty + \frac{k_a^{(1)}}{N} + \frac{k_a^{(2)}}{N^2} + \frac{k_e}{N^{\Delta_e+1}}, \tag{1.13}$$

$$m_N \sim m_\infty + \frac{u_a^{(1)}}{N} + \frac{u_a^{(2)}}{N^2} + \frac{u_e}{N^{\Delta_e+1}} \tag{1.14}$$

and

$$f_N \sim f_\infty + \frac{s_a^{(1)}}{N} + \frac{s_a^{(2)}}{N^2} + \frac{s_e}{N^{\Delta_e+1}} \tag{1.15}$$

respectively. The non-analytic correction to scaling exponent Δ_e is associated with the strongest non-analytic correction. One would expect further non-analytic (other Δ exponent-like terms) and analytic corrections (e.g. a N^{-2} term)—see [18] for a more in-depth discussion of possible scaling forms in general dimensions. Our numerical studies can discern only the strongest corrections to scaling. Again for the geometric size of the walk one may hypothesise that

$$R^2_{e,N} \sim d_e\, N^{2\nu} \left(1 + \frac{e_a}{N} + \frac{e_r}{N^{\Delta_r}}\right) \tag{1.16}$$

$$R^2_{m,N} \sim d_m\, N^{2\nu} \left(1 + \frac{o_a}{N} + \frac{o_r}{N^{\Delta_r}}\right) \tag{1.17}$$

with $2\nu = 1$ for $d \geq 5$.

It may be tempting in a non-rigorous treatment of SAW above the upper critical dimension to implicitly assume that the non-analytic corrections to scaling either do not occur or only occur with the same exponents as occur in RW. However, the field theoretic description of critical phenomena above the upper critical dimension is subtle (partially due to the presence of dangerously irrelevant variables) and mean-field theory is unlikely to be the whole story. For example, it is often assumed that hyperscaling relations break down above the upper critical dimension. On the other hand, it is widely accepted that the relation $2 - \alpha = d\nu$ holds for self-avoiding polygons in all dimensions, where $2 - \alpha$ is the entropic exponent associated p_N and ν is the size exponent, in seeming contradiction. It is certainly true that dominant exponents are usually not controlled by the fluctuation dominated critical behaviour that give rise to hyperscaling ($2 - \alpha \neq d\nu$ for the Ising model for $d > 4$) but rather mean-field energy vs entropy physics. However, it may be that remnants of the fluctuation driven critical behaviour still occur in high dimensions albeit now contributing to the corrections to scaling. In this picture the upper critical dimension d_u is the dimension below which fluctuation driven critical phenomena (characterised by hyperscaling relations) are dominant, while above d_u they are sub-dominant to mean-field criticality (fixed exponents). One hyperscaling relation expected to break down for $d \geq 5$ in SAW is $2\Delta_4 - \gamma = d\nu$ with the "gap" exponent Δ_4 associated with the "intersection" probability (see [18, 5] for example). One may be tempted to hypothesise a correction to the scaling to c_N of a term $\mu^N N^{2\Delta_4 - d\nu - 1}$. Since it is accepted that $\Delta_4 = 3/2$ (and proved that $\nu = 1/2$) we can hypothesise a correction to scaling exponent arising from such a term as

$$\Delta_e = \frac{(d-4)}{2}. \tag{1.18}$$

That is, in $d = 5$ we expect that $\Delta_e = 1/2$, so corrections of order $N^{-3/2}$ as well as analytic corrections of order N^{-1}, N^{-2} etc may occur. Unfortunately we are only practically able to detect corrections of order N^{-1} in our simulations and we have been unable to detect even the $N^{-3/2}$ in $d = 5$. We note in passing that there are predicted logarithmic corrections in $d = 4$ which we can see, to a similar extent as in [8], in our estimations of μ—in fact we have utilised this expected behaviour to give our refined estimation. We now comment that the non-analytic correction to scaling exponent hypothesised above is the same as the "crossover" exponent $\phi_e = (d-4)/2$ of the Edwards model. This leads us to conjecture that while there is strictly no crossover from Gaussian to non-Gaussian behaviour, the excluded volume could still make itself apparent in scaling through a scaling function in the variable bN^{ϕ_e}, where b is the bare measure of the excluded volume. We concede that a further assumption about the expansion of the scaling function is needed here. In any case following this line of argument it is then likely that such a correction to scaling term occurs in other quantities such as in the scaling of the size measures.

Assuming that the Edwards model crossover exponent provides the dominant corrections to scaling exponent for the size measures, $R^2_{e,N}$ and $R^2_{m,N}$, also gives us

$$\Delta_r = \Delta_e = \frac{(d-4)}{2}. \tag{1.19}$$

Hence in $d = 5$ we expect that $\Delta_r = 1/2$, and whenever the value of Δ_r coincides with an analytic correction to scaling (e.g. $d = 6$) there may also be confluent logarithms appearing. We have been able to successfully test for $\Delta_r = 1/2$ in $d = 5$ (see below), and we even have some evidence of confluent logarithms present for $d = 6$. One can also predict that for large N the quotients

$$B_N = R^2_{m,N}/R^2_{e,N} \sim B_\infty \left(1 + \frac{b_a}{N} + \frac{b_r}{N^{\Delta_r}}\right) \tag{1.20}$$

approach the random walk value, $B_\infty = d_m/d_e = \frac{1}{2}$ with the same type of corrections as the size measures approach their limits in $d \geq 5$. In conclusion, from the scaling forms above we predict that in $d = 5$ we generically expect to see, within the quality of data obtained, a correction of the order $N^{-1/2}$ in the size measure quantities. In dimensions 7 and 8 we expect to see only the N^{-1} corrections, while in $d = 6$ we may expect to see some confluent logarithmic correction term such as $\log(N)/N$.

Our simulations allow us to estimate μ, m_∞, f_∞, d_e (we certainly confirm that $d_e = 2d_m$ in all dimensions studied) and study the corrections to scaling in κ_N, m_N, $R^2_{e,N}$, $R^2_{m,N}$, B_N. Let us first discuss the constants as they provide the most important information contained in this paper. Our best estimates and various comparisons are provided in Tables 1, 2 and 3. We are able to compare our results to estimates and bounds from various sources. Fisher and Gaunt [19] used exact enumerations on general d-dimensional hypercubic lattices to give an asymptotic $1/d$-expansion for μ up to fifth order in the variable $s = (2d-1)$. Nemirovsky and Freed [20] extended this to include d_e, while Ishinabe *et al.* [21] extended it to include m_∞ and f_∞. In all these expansions the error is uncontrolled, and since they are considered asymptotic expansions the optimal number of terms to be used to give an accurate answer varies with dimension. All terms have been used when applied to $d \geq 5$ since Fisher and Gaunt [19] proposed that d terms plus half the next should be used in general. The $1/d$-expansions for μ, m_∞, f_∞, d_e, and d_m are

$$\mu = s - 1/s - 2/s^2 - 11/s^3 - 62/s^4 + \ldots \tag{1.21}$$

$$m_\infty = 1/s + 1/s^2 + 7/s^3 + 35/s^4 + 250/s^5 + \ldots \tag{1.22}$$

$$f_\infty = 1/s + 4/s^2 + 29/s^3 + 152/s^4 + 752/s^5 + \ldots \tag{1.23}$$

$$d_e = 1 + 2/s + 28/s^2 + 180/s^3 + 1382/s^4 + \ldots \tag{1.24}$$

where $s = (2d - 1)$ and the expansion for d_m is trivially given by half of the expansion for d_e. The specific values for $d = 4, \ldots, 8$ are given in Tables 1, 2 and 3. On the other hand, there has been much effort expended to obtain rigorous and (semi-)rigorous upper and lower bounds for the connective constants [11, 22, 23, 24, 25] in all dimensions. The lace expansion provides excellent lower bounds [11, 22] not only in high dimensions such as 5, 6, 7 and 8 but also in dimensions 3 and 4: lower bounds as quoted from Hara and Slade [11] for dimensions 4, 5 and 6, and for dimensions 7 and 8 have been computed via equation (2.34) of [11], are given in Table 1. The best current upper bounds [25, 24] are also listed in Tables 1, 2 and 3—the upper bounds for dimensions 7 and 8 have been computed using the Maple code available at [26]. We also include in our tables the previous most precise estimates. In dimensions 5, 6, 7 and 8 these have been from series analysis of exact enumeration data [6, 27, 28], while in dimension 4 the previous best estimate of μ was obtained by Grassberger [8]. The previous estimates for m_∞ are from exact enumerations and were given by Douglas and Ishinabe [28].

We now turn to our evidence for the types of corrections to scaling. For the entropy, mean number of contacts, and fluctuations in the mean number of contacts, we find that extrapolations assuming dominant $1/N$ corrections produce consistent extrapolates in all dimensions $d \geq 5$ and all lengths $N \geq 128$. Similarly for the size measure data, $R^2_{e,N}$, $R^2_{m,N}$ and B_N in dimensions $d = 7$ and $d = 8$ the assumption of $1/N$ corrections produces consistent extrapolates for all lengths $N \geq 128$. Thus we conclude that $1/N$ corrections dominate in those dimensions as predicted above.

The evidence for anomalous scaling is summarised in Figures 1 and 2: for $d = 5$, we clearly detect $N^{-1/2}$-corrections (see Figure 1) in the size measure data, and for $d = 6$ our results are suggestive of $N^{-1} \log N$-corrections, which produce a slightly better fit than N^{-1}-corrections (see Figure 2). We note in passing that the absence of $N^{-1/2}$-corrections in past extrapolations from exact enumeration data (see Table 3) may have affected previous estimates for A_e.

In summary, we have presented a comprehensive study of scaling of self-avoiding walks at and above the upper critical dimension, testing various scaling predictions and providing precise estimates of associated scaling amplitudes.

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dimension	4	5	6	7	8
estimate for μ	6.774043(5)	8.838544(3)	10.878094(4)	12.902817(3)	14.919257(2)
previous estimates [8, 6, 27]	6.77404(4)	8.8386(8)	10.8788(9)	12.900	14.920
lower bound[11]	6.7429	8.8285	10.8740	12.8811	14.9030
upper bound[25, 24]	6.8040	8.8602	10.8886	12.9081	14.9221
$1/d$-expansion[19]	6.7714	8.8397	10.8800	12.9040	14.9200

Table 1: *Numerical values for self-avoiding walk connective constants μ in dimension 4 to 8.*

dimension	4	5	6	7	8
estimate for m_∞	0.17088(5)	0.134576(6)	0.106902(4)	0.087715(2)	0.074222(2)
previous estimate[28]	0.1740(15)	0.141(1)	0.111(1)	0.0892(8)	0.0744(6)
$1/d$-expansion[28]	0.213125	0.142627	0.108376	0.087925	0.074206
estimate for f_∞	0.330(2)	0.2324(3)	0.1640(2)	0.12331(7)	0.09818(5)
$1/d$-expansion[28]	0.417	0.2362	0.1608	0.12114	0.09703

Table 2: *Numerical values for normalised mean m_∞ and fluctuation f_∞ of nearest-neighbour contacts in dimension 4 to 8.*

dimension	4	5	6	7	8
estimate for d_e	—	1.4767(13)	1.2940(6)	1.2187(3)	1.1760(2)
previous estimate[20]	—	1.434	1.296	1.222	1.178
$1/d$-expansion[20]	—	1.385	1.273	1.212	1.174
estimate for d_m	—	0.7385(6)	0.6470(2)	0.6094(1)	0.5880(1)
estimate for $B_\infty = d_m/d_e$	0.504(7)	0.5001(6)	0.5000(2)	0.5000(1)	0.5000(1)

Table 3: *Numerical values for distance amplitudes d_m and d_e and their quotient $B_\infty = d_m/d_e$ in dimension 4 to 8.*

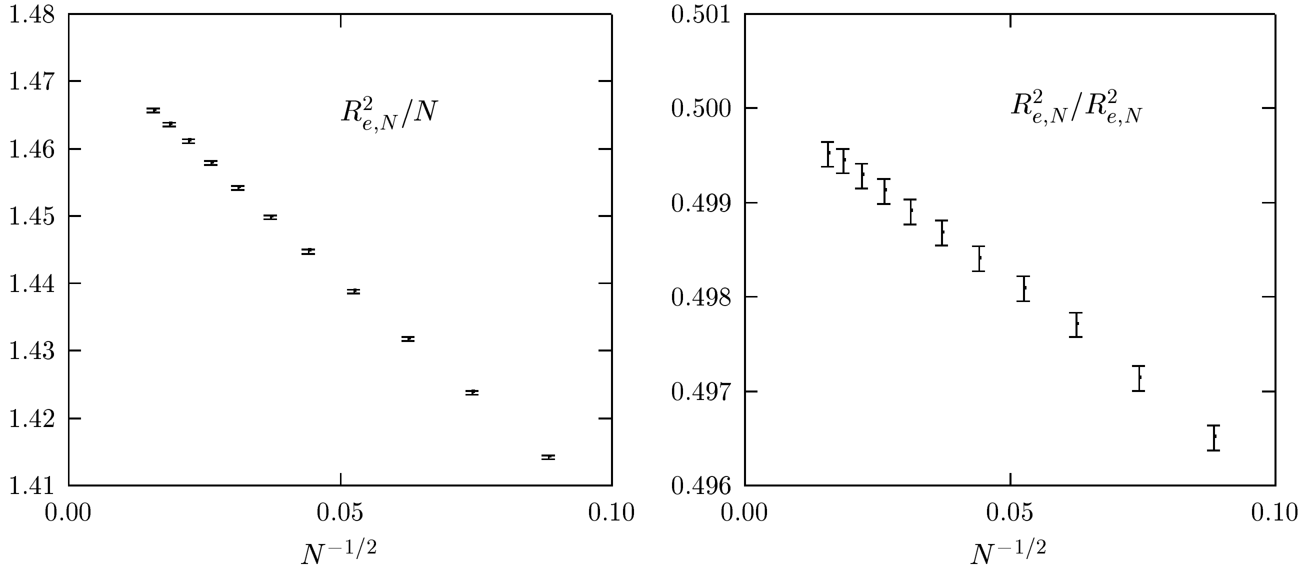

Figure 1: *$R^2_{e,N}/N$ and $B_N = R^2_{m,N}/R^2_{e,N}$ versus $N^{-1/2}$ for $d = 5$, showing clearly the presence of the $N^{-1/2}$-correction to scaling. From the right-hand-side plot we extrapolate $B_\infty = 0.5001(6)$.*

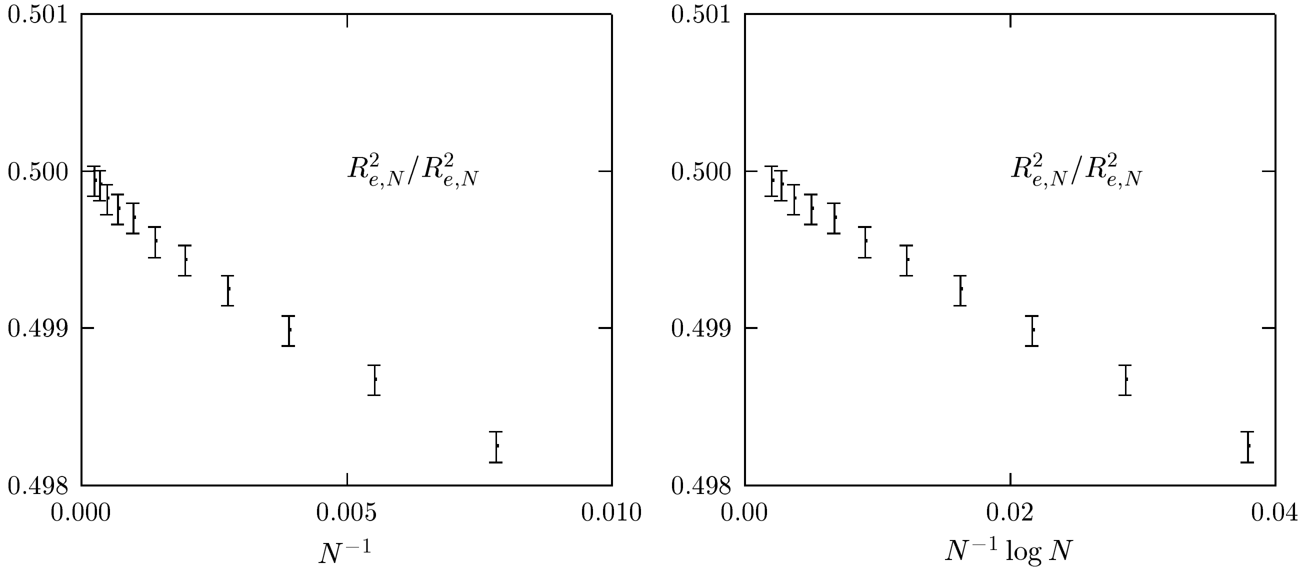

Figure 2: $B_N = R^2_{m,N}/R^2_{e,N}$ *versus* N^{-1} *and versus* $N^{-1}\log N$ *for* $d = 6$*, showing the possible presence of a confluent logarithm for the* N^{-1}*-correction to scaling. We extrapolate* $B_\infty = 0.5000(2)$*.*